Finite difference methods for the solution of the Schrödinger equation and related periodic problems

The Schrödinger equation has many important applications. Its nonlinear time-dependent form expresses atomic Bose–Einstein condensates, or light propagation in nonlinear optical beams. The linear time-independent form can provide, among others, estimates of the bound states, scattering states and resonances. In many interesting cases, the solutions have periodic/oscillatory behaviour, but without analytical solutions. Thus, numerical techniques are needed for the efficient solution of these problems.

Here, we present finite difference methods of different types, such as Runge-Kutta, Runge-Kutta-Nyström and linear multistep methods. These are optimised to solve the Schrödinger equation and related problems that exhibit periodic behaviour, such as the N-body problem. Techniques such as trigonometric fitting, phase fitting and amplification factor fitting are utilised. The conditions for the highest algebraic order are provided, and the intervals of stability and periodicity are studied. Methods with fixed or variable coefficients are produced and their efficiency is compared to other methods from the literature.